



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 5, 2020 – 04:33 am BST

PDB ID : 6CGV
Title : Revised crystal structure of human adenovirus
Authors : Natchiar, S.K.; Venkataraman, S.; Nemerow, G.R.; Reddy, V.S.
Deposited on : 2018-02-21
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

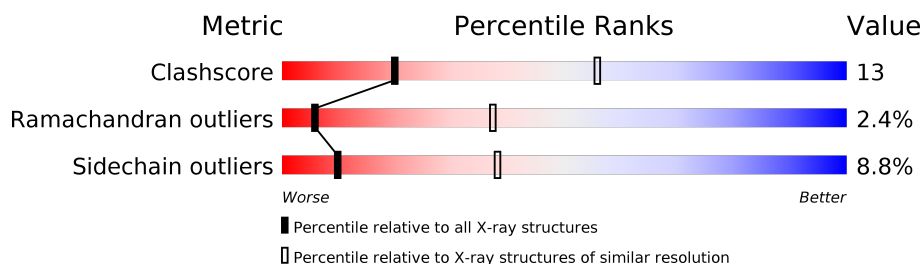
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	949	
1	B	949	
1	C	949	
1	D	949	
1	E	949	
1	F	949	
1	G	949	
1	H	949	

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Mol	Chain	Length	Quality of chain
1	I	949	 64%27%5% . .
1	J	949	 69%25%. . .
1	K	949	 66%25%. 5%
1	L	949	 69%23%. . .
2	N	571	 52%22%. 22%
3	M	585	 40%10%. 48%
4	P	140	 46%17%. 32%
4	Q	140	 69%21%. . 5%
4	R	140	 46%17%6%30%
4	S	140	 32%28%7%. 31%
5	U	227	 62%11%. 25%
5	V	227	 59%14%. . 23%
6	W	24	 46%46%. . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 99723 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	0	0
			7345	4668	1243	1400	34			
1	B	911	Total	C	N	O	S	0	0	0
			7295	4636	1235	1390	34			
1	C	921	Total	C	N	O	S	0	0	0
			7374	4686	1247	1405	36			
1	D	917	Total	C	N	O	S	0	0	0
			7345	4668	1243	1400	34			
1	E	910	Total	C	N	O	S	0	0	0
			7302	4645	1235	1388	34			
1	F	914	Total	C	N	O	S	0	0	0
			7325	4658	1239	1393	35			
1	G	909	Total	C	N	O	S	0	0	0
			7291	4636	1234	1387	34			
1	H	913	Total	C	N	O	S	0	0	0
			7317	4653	1238	1392	34			
1	I	917	Total	C	N	O	S	0	0	0
			7345	4669	1243	1398	35			
1	J	915	Total	C	N	O	S	0	0	0
			7329	4658	1240	1397	34			
1	K	904	Total	C	N	O	S	0	0	0
			7247	4606	1227	1380	34			
1	L	918	Total	C	N	O	S	0	0	0
			7353	4673	1244	1401	35			

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	447	Total	C	N	O	S	0	0	0
			3577	2264	621	680	12			

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	0
			2343	1447	430	460	6			

- Molecule 4 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	95	Total	C	N	O	S	0	0	0
			717	443	126	146	2			
4	Q	133	Total	C	N	O	S	0	0	0
			965	594	170	199	2			
4	R	98	Total	C	N	O	S	0	0	0
			734	450	132	150	2			
4	S	96	Total	C	N	O	S	0	0	0
			728	450	129	147	2			

- Molecule 5 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	171	Total	C	N	O	S	0	0	0
			1329	839	235	250	5			
5	V	174	Total	C	N	O	S	0	0	0
			1346	848	238	255	5			

- Molecule 6 is a protein called Pre-protein VI.

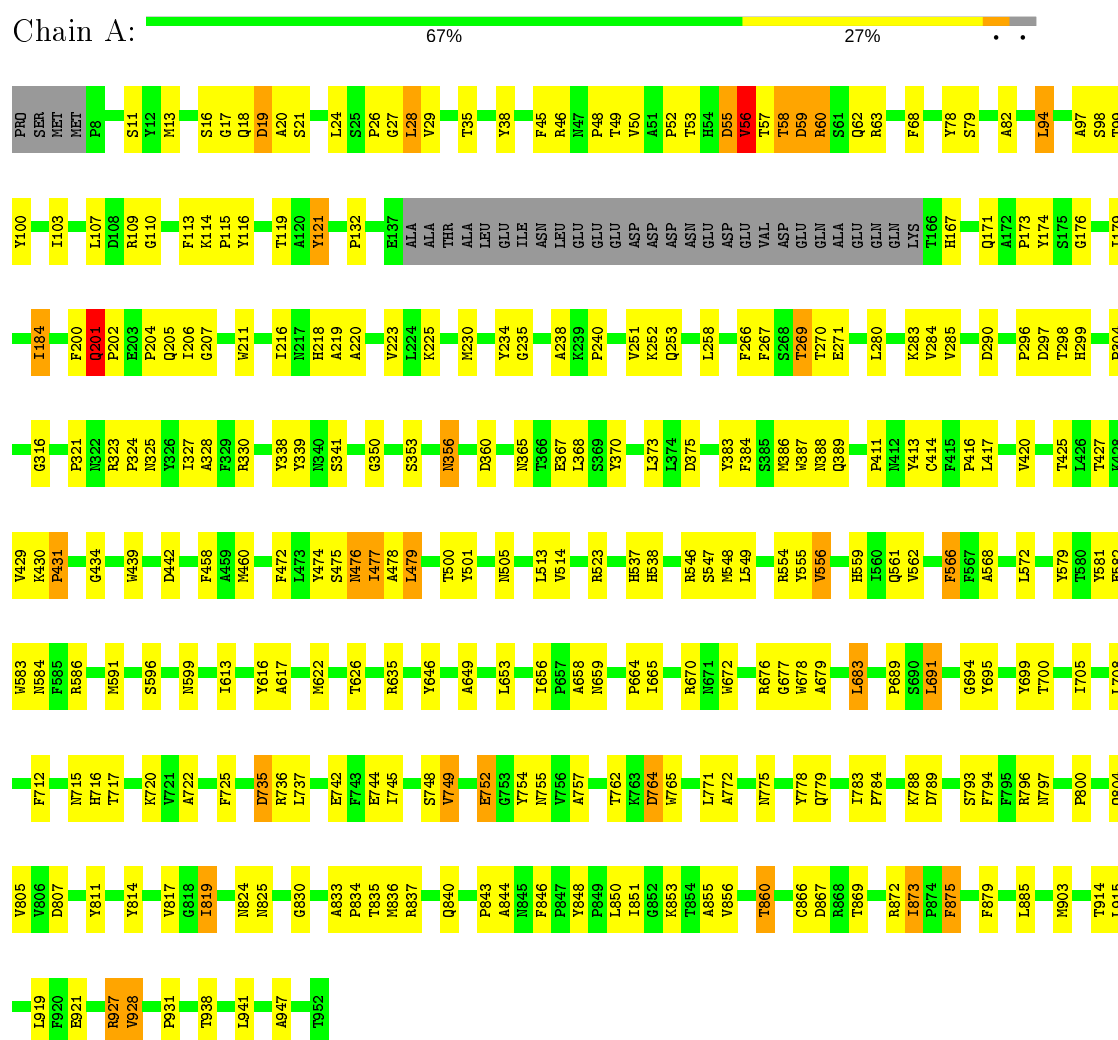
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	W	24	Total	C	N	O	0	0	0
			116	68	24	24			

3 Residue-property plots

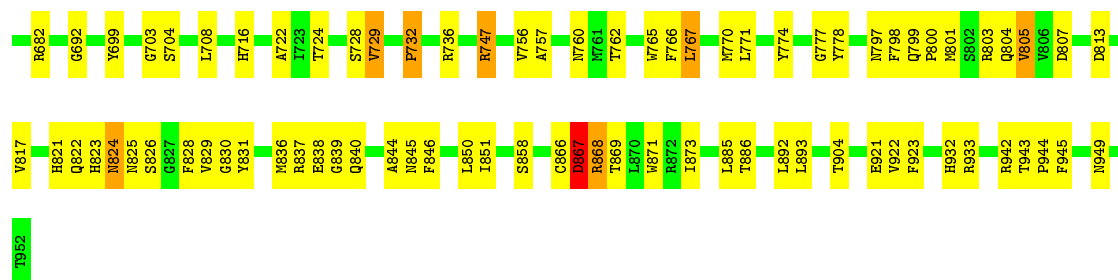
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

- Molecule 1: Hexon protein

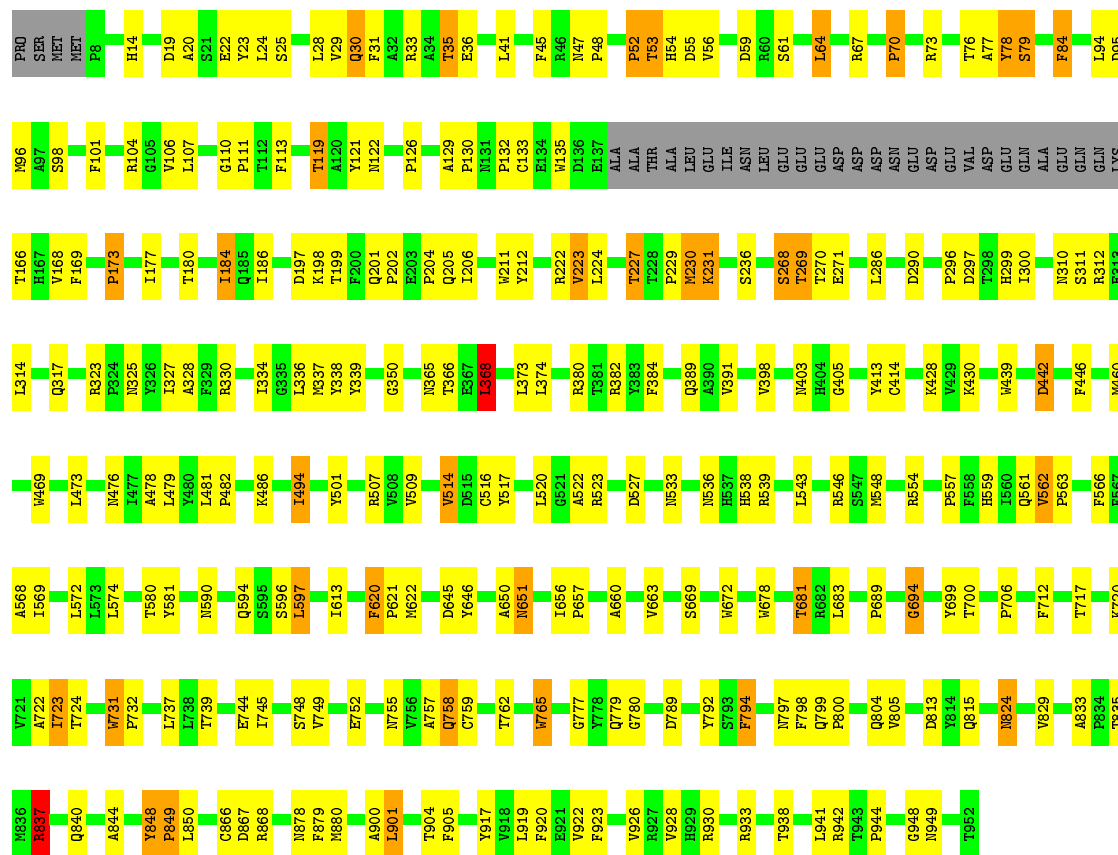






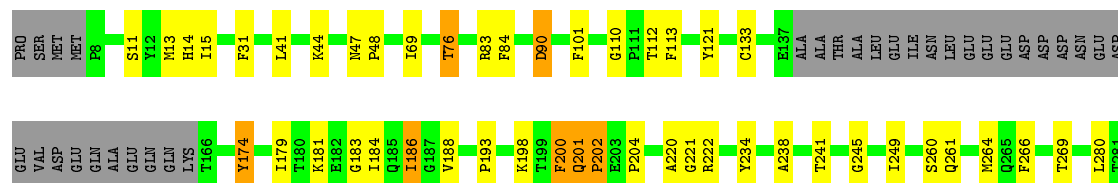
• Molecule 1: Hexon protein

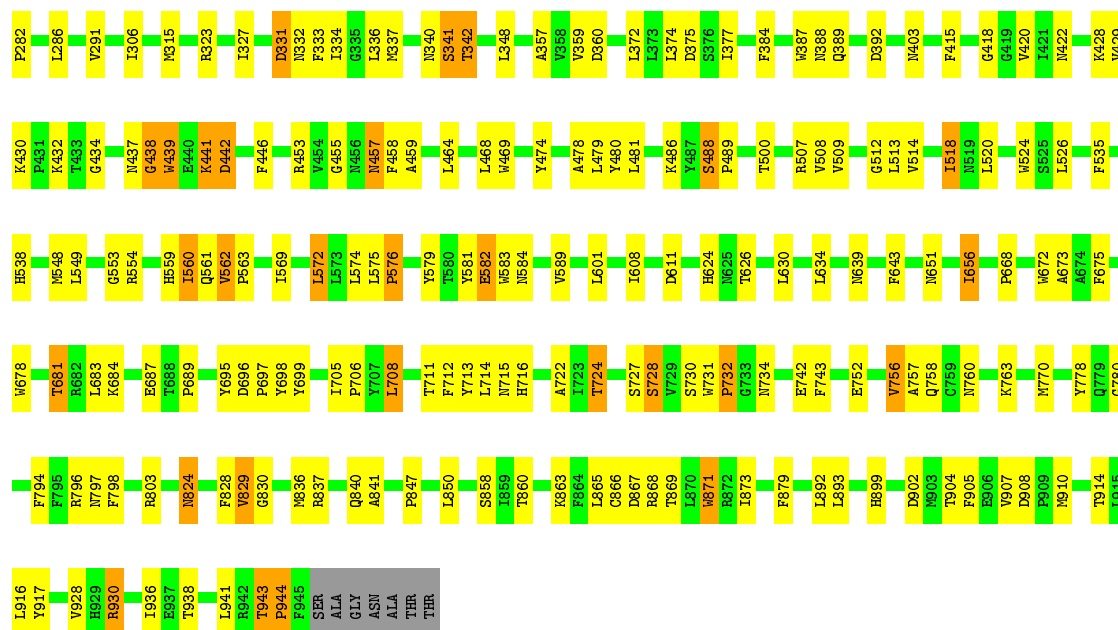
Chain D: 69% 24%



• Molecule 1: Hexon protein

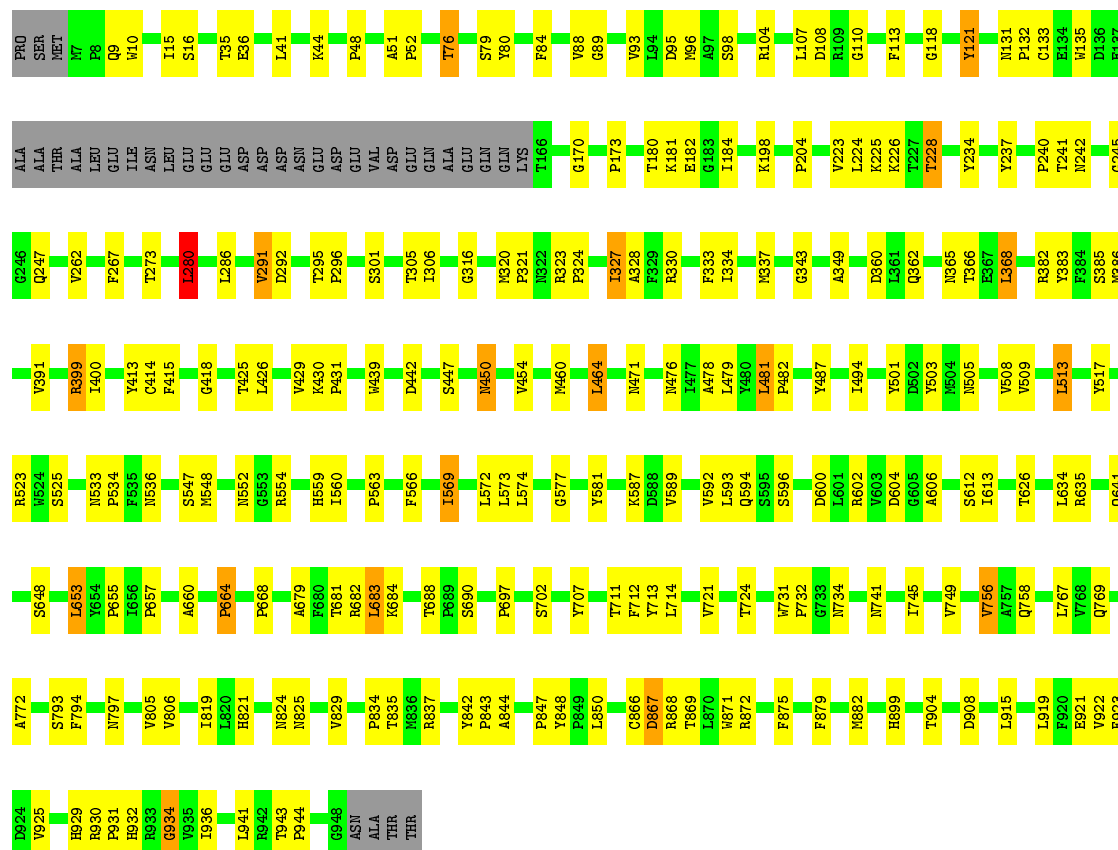
Chain E: 71% 22%





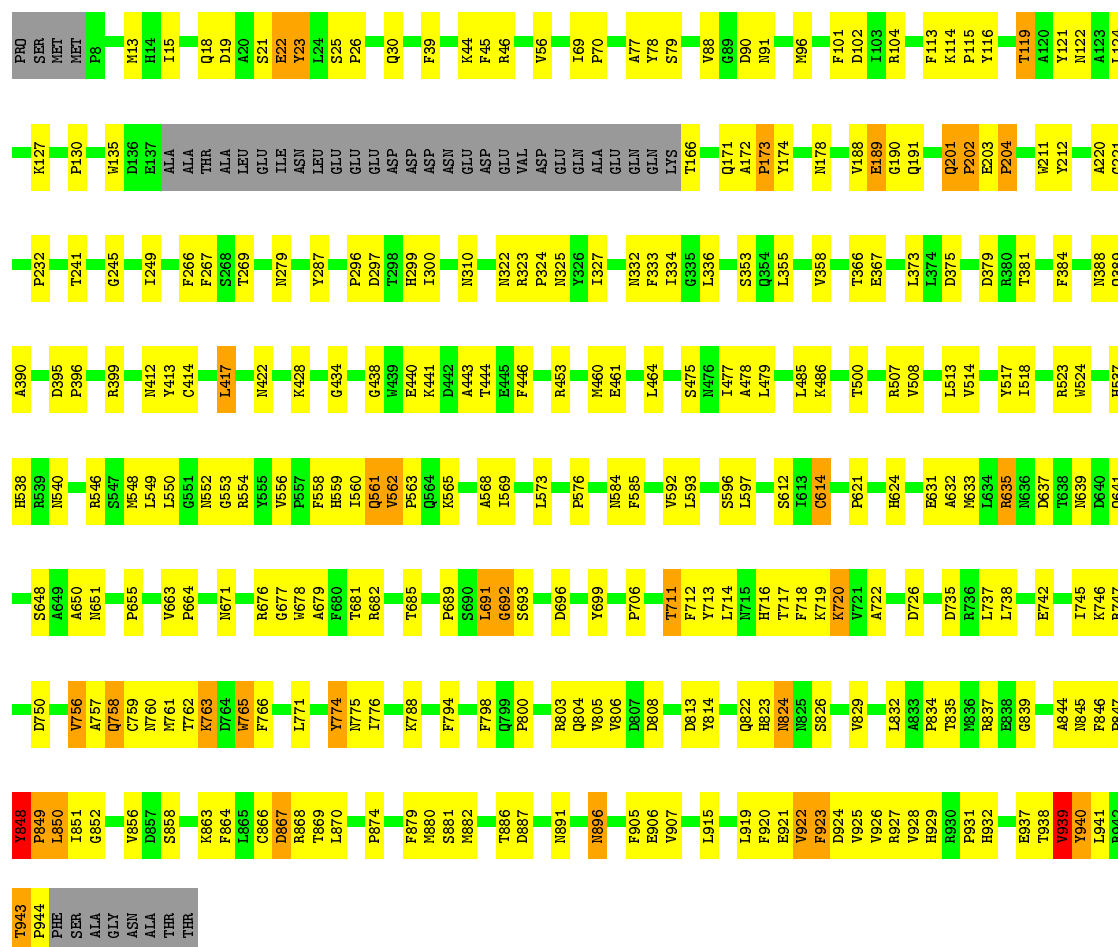
- Molecule 1: Hexon protein

Chain F: 72% 23%



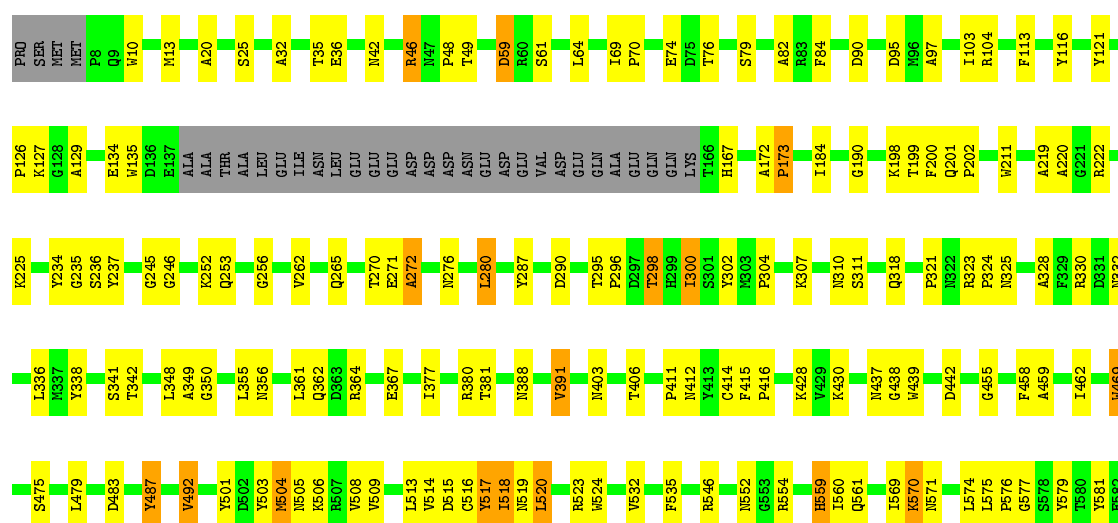
- Molecule 1: Hexon protein

Chain G: 

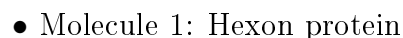


• Molecule 1: Hexon protein

Chain H: 

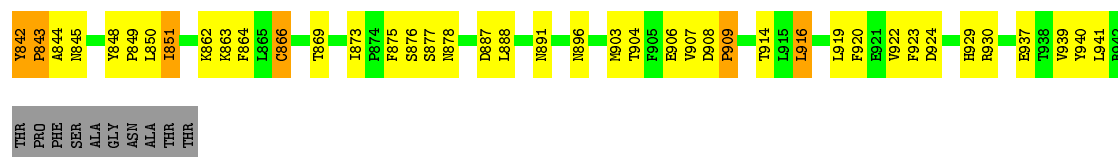




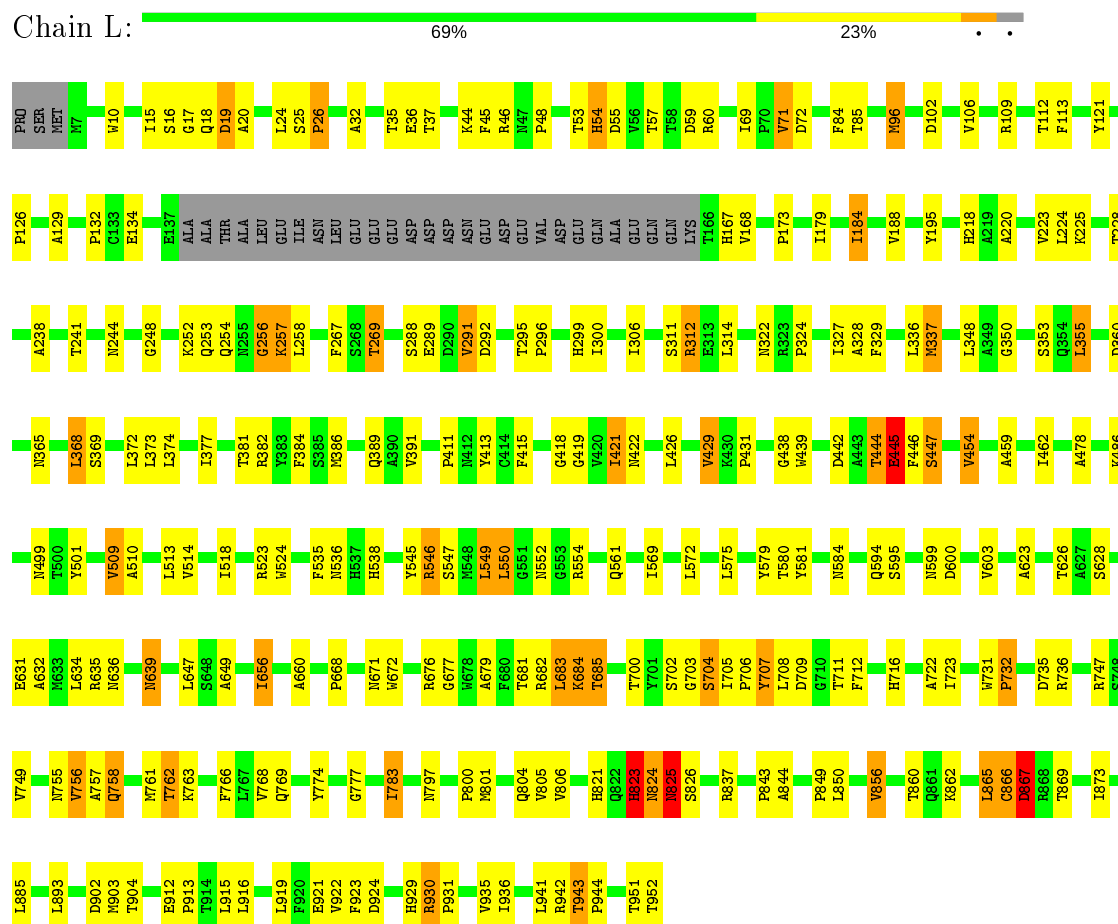


Device Type	Percentage
Smartphone	66%
Tablet	25%
Feature phone	5%





• Molecule 1: Hexon protein



F1	A2	S3	I4	A5	P6	R7	H8	G9	S10	R11	P12	F13	M16	W17	T22	S23	P24
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4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	854.25Å 855.32Å 865.91Å 60.38° 60.43° 61.98°	Depositor
Resolution (Å)	129.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (129.00-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.36	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.78Å)	Xtriage
Refinement program	REFMAC 5.8	Depositor
R, R_{free}	0.422 , 0.427	Depositor
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.080	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.226 for h-l,h,h-k 0.226 for k,k-l,-h+k 0.220 for h-k,h-l,h 0.220 for l,-h+l,-k+l 0.226 for -k+l,l,-h+l 0.226 for k-l,-h+k,k 0.220 for l,h,k 0.220 for k,l,h 0.226 for -l,k-l,h-l 0.226 for -h+l,-h+k,-h 0.220 for -k,h-k,-k+l 0.220 for -h+k,-h,-h+l 0.226 for h-k,-k+l,-k 0.226 for h-l,-l,k-l 0.226 for h,h-k,h-l 0.226 for -h+k,k,k-l 0.226 for -h,-l,-k 0.236 for -k,-h,-l 0.226 for k-l,h-l,-l 0.226 for -k+l,-k,h-k 0.226 for -h+l,-k+l,l 0.226 for -l,-k,-h 0.226 for -h,-h+l,-h+k	Xtriage

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¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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Property	Value	Source
Total number of atoms	99723	wwPDB-VP
Average B, all atoms (\AA^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/7543	0.77	12/10258 (0.1%)
1	B	0.49	0/7490	0.72	11/10185 (0.1%)
1	C	0.50	0/7573	0.72	8/10298 (0.1%)
1	D	0.48	1/7543 (0.0%)	0.71	11/10258 (0.1%)
1	E	0.46	0/7500	0.66	1/10200 (0.0%)
1	F	0.46	1/7523 (0.0%)	0.65	2/10231 (0.0%)
1	G	0.54	3/7488 (0.0%)	0.78	10/10184 (0.1%)
1	H	0.49	0/7515	0.74	7/10220 (0.1%)
1	I	0.52	1/7543 (0.0%)	0.77	11/10259 (0.1%)
1	J	0.46	0/7526	0.68	4/10235 (0.0%)
1	K	0.50	0/7440	0.73	5/10116 (0.0%)
1	L	0.50	0/7551	0.73	13/10269 (0.1%)
2	N	0.60	1/3663 (0.0%)	0.87	9/4989 (0.2%)
3	M	0.46	0/2380	0.70	2/3240 (0.1%)
4	P	0.78	4/726 (0.6%)	0.96	4/989 (0.4%)
4	Q	0.78	2/977 (0.2%)	1.00	4/1333 (0.3%)
4	R	0.67	2/741 (0.3%)	0.97	3/1006 (0.3%)
4	S	1.08	4/736 (0.5%)	1.26	4/1000 (0.4%)
5	U	0.43	0/1367	0.63	0/1868
5	V	0.53	0/1384	0.72	2/1891 (0.1%)
6	W	0.80	0/115	1.29	2/157 (1.3%)
All	All	0.51	19/102324 (0.0%)	0.74	125/139186 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
3	M	0	1
All	All	0	2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	56	PRO	CA-C	9.69	1.72	1.52
4	Q	55	THR	C-N	9.24	1.51	1.34
4	S	56	PRO	C-N	8.73	1.54	1.34
4	P	6	PHE	N-CA	8.02	1.62	1.46
4	S	57	LEU	N-CA	7.83	1.62	1.46

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	23	TYR	CB-CG-CD1	-15.65	111.61	121.00
1	G	23	TYR	CB-CG-CD2	15.43	130.25	121.00
1	D	78	TYR	CB-CG-CD2	-10.26	114.84	121.00
4	R	6	PHE	CB-CG-CD2	9.83	127.68	120.80
1	B	532	VAL	CB-CA-C	-9.69	92.98	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	501	TYR	Sidechain
3	M	106	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7345	0	7042	232	0
1	B	7295	0	6999	224	0
1	C	7374	0	7074	188	0
1	D	7345	0	7045	166	0
1	E	7302	0	7006	150	0
1	F	7325	0	7027	133	0
1	G	7291	0	6997	254	0
1	H	7317	0	7019	237	0
1	I	7345	0	7045	262	0
1	J	7329	0	7028	201	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	7247	0	6957	211	0
1	L	7353	0	7052	195	0
2	N	3577	0	3508	145	0
3	M	2343	0	2313	52	0
4	P	717	0	724	39	0
4	Q	965	0	971	56	0
4	R	734	0	741	27	0
4	S	728	0	739	59	0
5	U	1329	0	1290	18	0
5	V	1346	0	1302	19	0
6	W	116	0	54	21	0
All	All	99723	0	95933	2464	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2464 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:698:TYR:CE1	4:Q:24:GLY:HA2	1.10	1.58
1:H:698:TYR:HE1	4:Q:24:GLY:CA	1.19	1.54
4:P:40:LEU:HB2	4:P:41:PRO:CD	1.44	1.46
1:A:18:GLN:HB2	6:W:10:SER:CB	1.30	1.46
6:W:7:ARG:CB	6:W:11:ARG:O	1.65	1.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	913/949 (96%)	749 (82%)	143 (16%)	21 (2%)	6 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	907/949 (96%)	748 (82%)	130 (14%)	29 (3%)	4	32
1	C	917/949 (97%)	745 (81%)	149 (16%)	23 (2%)	5	36
1	D	913/949 (96%)	766 (84%)	124 (14%)	23 (2%)	5	36
1	E	906/949 (96%)	752 (83%)	138 (15%)	16 (2%)	8	42
1	F	910/949 (96%)	748 (82%)	144 (16%)	18 (2%)	7	41
1	G	905/949 (95%)	738 (82%)	144 (16%)	23 (2%)	5	36
1	H	909/949 (96%)	747 (82%)	140 (15%)	22 (2%)	6	37
1	I	913/949 (96%)	756 (83%)	125 (14%)	32 (4%)	3	31
1	J	911/949 (96%)	751 (82%)	149 (16%)	11 (1%)	13	50
1	K	900/949 (95%)	735 (82%)	145 (16%)	20 (2%)	6	39
1	L	914/949 (96%)	759 (83%)	131 (14%)	24 (3%)	5	36
2	N	443/571 (78%)	352 (80%)	77 (17%)	14 (3%)	4	32
3	M	301/585 (52%)	263 (87%)	32 (11%)	6 (2%)	7	41
4	P	91/140 (65%)	74 (81%)	15 (16%)	2 (2%)	6	39
4	Q	131/140 (94%)	113 (86%)	15 (12%)	3 (2%)	6	38
4	R	94/140 (67%)	81 (86%)	11 (12%)	2 (2%)	7	40
4	S	92/140 (66%)	73 (79%)	15 (16%)	4 (4%)	2	26
5	U	167/227 (74%)	141 (84%)	22 (13%)	4 (2%)	6	37
5	V	170/227 (75%)	138 (81%)	26 (15%)	6 (4%)	3	31
6	W	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2	25
All	All	12429/13582 (92%)	10248 (82%)	1877 (15%)	304 (2%)	6	37

5 of 304 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	271	GLU
1	A	388	ASN
1	B	417	LEU
1	B	570	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	799/827 (97%)	740 (93%)	59 (7%)	13	44
1	B	794/827 (96%)	739 (93%)	55 (7%)	15	46
1	C	803/827 (97%)	741 (92%)	62 (8%)	13	43
1	D	799/827 (97%)	738 (92%)	61 (8%)	13	43
1	E	795/827 (96%)	721 (91%)	74 (9%)	9	35
1	F	797/827 (96%)	729 (92%)	68 (8%)	10	40
1	G	794/827 (96%)	722 (91%)	72 (9%)	9	36
1	H	796/827 (96%)	736 (92%)	60 (8%)	13	44
1	I	799/827 (97%)	709 (89%)	90 (11%)	6	28
1	J	797/827 (96%)	724 (91%)	73 (9%)	9	35
1	K	789/827 (95%)	711 (90%)	78 (10%)	8	32
1	L	800/827 (97%)	732 (92%)	68 (8%)	10	40
2	N	404/489 (83%)	366 (91%)	38 (9%)	8	35
3	M	253/500 (51%)	235 (93%)	18 (7%)	14	45
4	P	84/112 (75%)	74 (88%)	10 (12%)	5	26
4	Q	106/112 (95%)	96 (91%)	10 (9%)	8	35
4	R	84/112 (75%)	67 (80%)	17 (20%)	1	9
4	S	84/112 (75%)	69 (82%)	15 (18%)	2	12
5	U	144/186 (77%)	132 (92%)	12 (8%)	11	40
5	V	145/186 (78%)	130 (90%)	15 (10%)	7	31
All	All	10866/11733 (93%)	9911 (91%)	955 (9%)	10	38

5 of 955 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	776	ILE
1	I	336	LEU
4	P	39	VAL
1	G	887	ASP
1	H	559	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 228 such

sidechains are listed below:

Mol	Chain	Res	Type
1	G	538	HIS
1	H	412	ASN
2	N	174	ASN
1	G	559	HIS
1	G	804	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.